SCIEX

Answers for Science.
Knowledge for Life.™

Case Study

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Project Goal

To achieve the global identification of metabolomes including bacteria, plant, human host, microbiota, and exposome compounds. This is achieved by advancements in analytical chemistry and informatics, mainly focusing on the computational science.

The Challenges

- Developing a universal software program for handling metabolomics data from infusion, ion mobility, and conventional chromatography/mass spectrometry data
- Linking to genomics, transcriptomics, and proteomics from the new discovery of metabolites
- Improving the coverage of metabolomics and lipidomics, especially for natural products and microbiota metabolites

The Solution

- Creating data processing software programs to efficiently extract metabolite ion features
- Formulating the relationship between metabolite structures and mass fragmentations using enriched mass spectral databases
- Creating new algorithms for predicting molecular formula, metabolite class (ontology), and structure

The Outcomes

- 12 informatics tools including MS-DIAL, MS-FINDER, and MRMPROBS that are published in "Computational metabolomics" section in RIKEN PRIMe (http://prime.psc.riken.jp).

Type of Organization

A comprehensive research institution renowned for basic and applied sciences, and a world leader in a diverse array of scientific disciplines.

Goals

To achieve the global identification of metabolomes in various living organisms by creating novel methodologies in mass spectrometry and computational sciences.

SCIEX Products

- TripleTOF® 6600 system
- TripleTOF® 5600 system
- QTRAP® 5500 LC-MS/MS
- QTRAP® 4500 LC-MS/MS

Computational mass spectrometry deepens the understanding of metabolism

"Decoding mass spectrometry data leads to new discovery in small molecule (metabolomics) research, and we have to understand the physical/ chemical phenomena of ionized metabolites as a big data science."